

Refinement trajectory and determination of eigenstates by a wavelet based adaptive method

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The detail structure of the wave function is analyzed at various refinement levels using the methods of wavelet analysis. The eigenvalue problem of a model system is solved in granular Hilbert spaces, and the trajectory of the eigenstates is traced in terms of the resolution. An adaptive method is developed for identifying the fine structure localization regions, where further refinement of the wave function is necessary.

I. INTRODUCTION

Multiresolution or wavelet analysis (MRA) [1, 2] is increasingly used in advanced data compression and image coding algorithms [3], and several promising approaches applied this technique in describing electronic structures. Arias *et al.* [4] elaborated a Kohn-Sham equation based *density functional* (DFT) method, Goedecker and Ivanov [5] have also successfully used wavelets for the solution of Poisson's equation. There are also attempts to extend wavelet calculations to three dimensional structures in a computationally manageable manner [6].

The basic principle of the application of MRA is the recognition that the details of the electronic structure are not distributed equally over different parts of the system. In data compression the details of the picture are systematically included by consecutive refinements of the image only in those spatial regions where it is necessary. A similar approach to the electronic wave function suggests that the fine details of the distribution are concentrated around the nuclear cusps and singularities of the two-electron density matrix. It has been shown, that the surroundings of a molecule can be described at a rather rough resolution level [7]. We have also demonstrated [8], that the extremely hardly representable electron-electron cusp singularity of the two-electron density operator can be easily reproduced by the method of multiresolution analysis.

The applicability of these approaches strongly depends on the necessary depth of refinement. Clearly, a uniform refinement of the distributions leads to an exponential increase of the computational efforts with growing resolution level. The region where the refinements are applied has to be confined, in order to achieve computationally manageable algorithms. In this contribution we study

some questions concerning several aspects raised by the above considerations. We analyze the detail structure of the wave function, we explore how the spatial regions where further refinement is necessary are to be identified, and how can the extension of the eigenvalue problem to new subspaces be restricted. We trace how the projection of the wave function to different resolution level subspaces is changing in the course of the consecutive refinement steps. The performance of the adaptive refinement algorithm is tested by numerical comparisons to the exact analytical solution of the harmonic oscillator.

II. RESOLUTION STRUCTURE OF THE HILBERT SPACE

Multiresolution analysis theory ensures that an arbitrary element of the Hilbert space $\Psi \in \mathcal{H}$ can be exactly decomposed into orthogonal components as

$$\Psi(x) = \sum_{\ell \in \mathbb{Z}} c_{\ell} s_{0\ell}(x) + \sum_{m=0}^{\infty} \sum_{\ell \in \mathbb{Z}} d_{m\ell} w_{m\ell}(x). \quad (1)$$

Here, the basis functions $s_{0\ell}(x) = s_0(x - \ell)$ are equidistant shifts of the “mother scaling function” s_0 over a coarse grid of spacing 1. Refinements to the first approximation described by the first summation in (1) are introduced by the $m = 0$ level wavelets $w_{0\ell}(x) = w_0(x - \ell)$. The “mother wavelet” w_0 is orthogonal to s_0 , and generally, $\langle s_{0\ell} | s_{0k} \rangle = \delta_{\ell k}$, $\langle s_{0\ell} | w_{0k} \rangle = 0$ and $\langle w_{0\ell} | w_{0k} \rangle = \delta_{\ell k}$. Further refinements are expanded by the basis vectors $w_{m\ell}(x) = 2^{m/2} w_0(2^m x - \ell)$ for resolution levels $m = 1, 2, \dots$, with the orthogonality relations $\langle s_{0\ell} | w_{mk} \rangle = 0$ and $\langle w_{m\ell} | w_{jk} \rangle = \delta_{mj} \delta_{\ell k}$. The subspaces

$V_0 = \text{span}\{s_{0\ell} | \ell \in \mathbb{Z}\}$, $W_m = \text{span}\{w_{m\ell} | \ell \in \mathbb{Z}\}$ constitute a complete decomposition of the Hilbert space

$$\mathcal{H} = V_0 \oplus W_0 \oplus W_1 \oplus \dots, \quad (2)$$

i.e., expansion (1) is exact.

We define the resolution structure of the wave function by the series of components

$$\begin{aligned} P_0\Psi &= \sum_{\ell \in \mathbb{Z}} c_\ell s_{0\ell} \\ Q_0\Psi &= \sum_{\ell \in \mathbb{Z}} d_{0\ell} w_{0\ell} \\ Q_1\Psi &= \sum_{\ell \in \mathbb{Z}} d_{1\ell} w_{1\ell}, \\ &\vdots \end{aligned} \quad (3)$$

where P_0 and Q_m are orthogonal projection operators to subspaces V_0 and W_m , respectively. As according to Parseval's equality

$$\|P_0\Psi\|^2 + \sum_{m=0}^{\infty} \|Q_m\Psi\|^2 = 1, \quad (4)$$

we can measure the m th level complexity of the wave function by the number $\|Q_m\Psi\|^2$, which characterizes how important is the detail space W_m in expanding Ψ .

The decision, to include or omit W_m is crucial in developing useful algorithms for the following reasons. The basis functions of W_m are "sitting" on an equidistant grid with a grid length of $\sim 2^{-m}$. If a function constrained to a finite domain of the space is expanded, the number of basis functions in W_m is increasing like $\sim 2^{mD}$, where D is the dimension of the system. This exponential "explosion" makes the direct application of (1) unacceptable. Detail spaces with negligible $\|Q_m\Psi\|^2$ (lower than a predefined threshold) can be completely ignored. The experience [7, 9] of finding details in a constrained region of the space leads, however, to the conclusion, that even if

$$\|Q_m\Psi\|^2 = \sum_{\ell \in \mathbb{Z}} d_{m\ell}^2 \quad (5)$$

is significant, only very few terms in the summation contribute essentially to its value. This recognition would help to avoid the exponential explosion mentioned above, by using the restricted detail space $\widetilde{W}_m = \text{span}\{w_{m\ell} | \text{where } d_{m\ell} \text{ is significant}\}$.

The outlined strategy is, however, useless, if the choice of the significant $d_{m\ell}$ would be based on a prior calculation of *all* coefficients, and testing how many $d_{m\ell}$ are necessary to fulfill (5) with a good approximation. Clearly, a predictive method is needed.

A. Decomposition of exact wave functions

We will illustrate the above consideration with a simple exactly solvable example in $D = 1$ dimension. The

case of $D = 3$ is expected to have similar behavior with correspondingly greater numbers of basis functions. The ground state and some excited states of the standard example of the 1D harmonic oscillator with the Hamiltonian

$$H = -\frac{1}{2}\nabla^2 + \frac{\omega^2}{2}x^2 \quad (6)$$

are analyzed. One reason for choosing this system is that the matrix elements $\langle s_{0\ell} | H | s_{0k} \rangle$, $\langle s_{0\ell} | H | w_{jk} \rangle$ and $\langle w_{m\ell} | H | w_{jk} \rangle$ can be calculated exactly for (6), making possible to avoid inaccuracies not connected to Hilbert space constraints. The grid length of the scaling function subspace V_0 was set to 1 a.u. The expansion coefficients were calculated as

$$c_\ell = \langle s_{0\ell} | \Psi \rangle \quad \text{and} \quad d_{m\ell} = \langle w_{m\ell} | \Psi \rangle, \quad (7)$$

where Ψ stands for the exact ground or excited state wave function. The Daubechies-6 [1] set was chosen for the multiresolution basis set $\{s_{0\ell}, w_{m\ell}\}$. The elements of this set have finite support (the mother scaling function is zero outside of the interval $[0, 5)$), and both the scaling functions and the wavelets are differentiable. The scalar products in (7) were numerically calculated on a grid of 2^{-15} a.u. density. Fig. 1 shows the values $\|Q_m\Psi_i\|^2$ for various excitations $i = 0, \dots, 5$ with $\omega = 1$, whereas the projections to the scaling function subspace are given as follows: $\|P_0\Psi_0\|^2 = 0.9972$, $\|P_0\Psi_1\|^2 = 0.9822$, $\|P_0\Psi_2\|^2 = 0.9561$, $\|P_0\Psi_3\|^2 = 0.8637$, $\|P_0\Psi_4\|^2 = 0.9362$ and $\|P_0\Psi_5\|^2 = 0.5582$. It

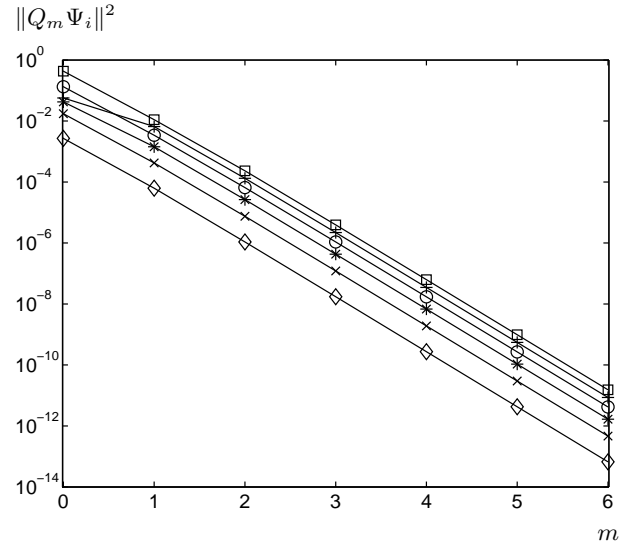


FIG. 1: The amplitudes of the projections of the exact eigenfunctions of the Hamiltonian (6) with $\omega = 1$ to the detail spaces W_m for $m = 0, \dots, 6$. The sign \diamond stands for the ground state $i = 0$, whereas the signs \times , $*$, \circ , $+$ and \square denote the excitations $i = 1, 2, 3, 4, 5$, respectively. Atomic units are used.

is clear, that the bulk of the states is described at level $m = 0$, and the contributions of the detail spaces disappear with increasing m . It is important to realize, that

even if the number of basis functions in subspace W_m increases as $\sim 2^m$, the *total contribution* of the subspace to the wave function exponentially decreases. This results coincides with our previous statement [10] that many-electron density operators can not contain arbitrary fine (nor rough) details.

B. Fine structure localization

Besides a “vertical” truncation of the Hilbert space over a sufficiently large resolution level M , there is a possibility of reducing the size of the subspaces W_m in a “horizontal” truncation process, by decimating the basis functions $w_{m\ell}$ which belong to those spatial regions where the wave function does not contain fine details.

In order to study the extent of this fine structure localization, we have also examined, how many coefficients c_ℓ and $d_{m\ell}$ are essential in the norms $\|P_0\Psi_i\|^2$ and $\|Q_m\Psi_i\|^2$, respectively. The projections of the wave function to the restricted subspaces \tilde{W}_0 and \tilde{W}_m are defined by the projectors \tilde{P}_0 and \tilde{Q}_m .

After numerically calculating the scalar products (7), a threshold value η , close to 1 was chosen. We counted the number $\#\tilde{W}_0$ and $\#\tilde{W}_m$ of most significant coefficients for which the inequalities

$$\begin{aligned} \|P_0\Psi_i\|^2 - \|\tilde{P}_0\Psi_i\|^2 &\leq 1 - \eta \quad \text{and} \\ \|Q_m\Psi_i\|^2 - \|\tilde{Q}_m\Psi_i\|^2 &\leq 1 - \eta \end{aligned} \quad (8)$$

hold. This criterion allows each subspace W_m to introduce an error $1 - \eta$ uniformly, and for those m where $\|Q_m\Psi_i\|^2 \leq 1 - \eta$ the complete subspace can be omitted, thus $\tilde{W}_m = \emptyset$. Fig. 2 summarizes the results for the ground and a selected excited state as a function of η for various resolution levels. On the horizontal axes the number of digit 9 in η is shown, i.e., the value 1 corresponds to $\eta = 0.9$, whereas 5 corresponds to $\eta = 0.99999$, etc. It is clearly seen, that ground and excited states behave in a very similar manner. As the logarithmic plots show, in the $\eta \rightarrow 1$ limit the number of basis functions in the subspaces W_m increases as $\sim 2^m$. On the other hand, if a finite, but even relatively high precision, like $\eta = 0.9999999999$ is demanded, many of the high resolution detail spaces drop out, and even at lower resolution m , only an acceptable amount of basis functions contribute to the truncated subspaces.

III. TRAJECTORY AND LIMITING BEHAVIOR OF THE EIGENFUNCTIONS IN COARSE-GRAINED HILBERT SPACES

In applied calculations the granularity M of the Hilbert space (i.e., the maximum resolution m in the summations of (1) and (4)) can not be arbitrary large. Instead, for a finite granularity M the eigenvalue problem is solved in

the restricted Hilbert space

$$\mathcal{H}^{[M]} = V_0 \oplus W_0 \oplus W_1 \oplus \cdots \oplus W_{M-1}, \quad (9)$$

which assumption seems to be warranted in the light of the above results. For $M = 0$, we define $\mathcal{H}^{[0]} = V_0$. The solution of the eigenvalue problem of H in the coarse-grained Hilbert space $\mathcal{H}^{[M]}$ leads to the ground and excited states $\Psi_i^{[M]}$ ($i = 0, 1, 2, \dots$). In this case we lose fine details, thus the natural question arises, how the trajectory $\Psi_i^{[0]} \rightarrow \Psi_i^{[1]} \rightarrow \Psi_i^{[2]} \rightarrow \cdots$ approaches the limit Ψ_i .

We have determined the eigenfunctions of the Hamiltonian (6) with $\omega = 1$ for $M = 0, \dots, 5$. In order to keep the number of basis functions finite, the spatial extension of the system has to be limited. We have chosen $|x| \leq x_{\max} = 10$ in (6). The error made by this assumption can be estimated by the omitted part of the norm square of the ground state

$$1 - \int_{-x_{\max}}^{x_{\max}} |\Psi_0|^2 dx = 1 - \text{erf}(\sqrt{\omega} x_{\max})$$

which is less than the accuracy of the double precision numerical representation.

The four-index matrix elements of H can be reduced to two-index quantities by a simple variable transformation. The kinetic energy matrix elements are calculated using the fact that the momentum operator is self-adjoint, thus for $m_1 \leq m_2$

$$\begin{aligned} \langle s_{0\ell_1} | -\nabla^2/2 | s_{0\ell_2} \rangle &= 2^{-1} \langle s'_{00} | s'_{0\ell_2-\ell_1} \rangle, \\ \langle s_{0\ell_1} | -\nabla^2/2 | w_{m_2\ell_2} \rangle &= 2^{-1} \langle s'_{00} | w'_{m_2 L} \rangle, \\ \langle w_{m_1\ell_1} | -\nabla^2/2 | w_{m_2\ell_2} \rangle &= 2^{2m_1-1} \langle w'_{00} | w'_{m_2-m_1 L} \rangle, \end{aligned} \quad (10)$$

with $L = \ell_2 - 2^{m_2-m_1}\ell_1$. The potential energy matrix elements are

$$\begin{aligned} \langle s_{0\ell_1} | \omega^2 x^2/2 | s_{0\ell_2} \rangle &= \omega^2 2^{-1} (\langle s_{00} | x^2 | s_{0\ell_2-\ell_1} \rangle \\ &\quad + 2\ell_1 \langle s_{00} | x | s_{0\ell_2-\ell_1} \rangle \\ &\quad + \ell_1^2 \langle s_{00} | s_{0\ell_2-\ell_1} \rangle), \\ \langle s_{0\ell_1} | \omega^2 x^2/2 | w_{m_2\ell_2} \rangle &= \omega^2 2^{-1} (\langle s_{00} | x^2 | w_{m_2 L} \rangle \\ &\quad + 2\ell_1 \langle s_{00} | x | w_{m_2 L} \rangle \\ &\quad + \ell_1^2 \langle s_{00} | w_{m_2 L} \rangle), \\ \langle w_{m_1\ell_1} | \omega^2 x^2/2 | w_{m_2\ell_2} \rangle &= \omega^2 2^{-2m_1-1} \cdot \\ &\quad (\langle w_{00} | x^2 | w_{m_2-m_1 L} \rangle \\ &\quad + 2\ell_1 \langle w_{00} | x | w_{m_2-m_1 L} \rangle \\ &\quad + \ell_1^2 \langle w_{00} | w_{m_2-m_1 L} \rangle). \end{aligned} \quad (11)$$

At any resolution level, the x^2 and x operators can be exactly expanded as linear combinations of scaling functions [1]. Wavelets are also finite linear combinations of scaling functions of the succeeding resolution level. Consequently, the remaining part of the calculation contains the evaluation of integrals of type $\int s_{\mu_1\lambda_1}(x)s_{\mu_2\lambda_2}(x)s_{\mu_3\lambda_3}(x)dx$ with $s_{\mu\lambda}(x) = 2^{\mu/2}s_0(2^\mu x - \lambda)$. There exist special algorithms for this

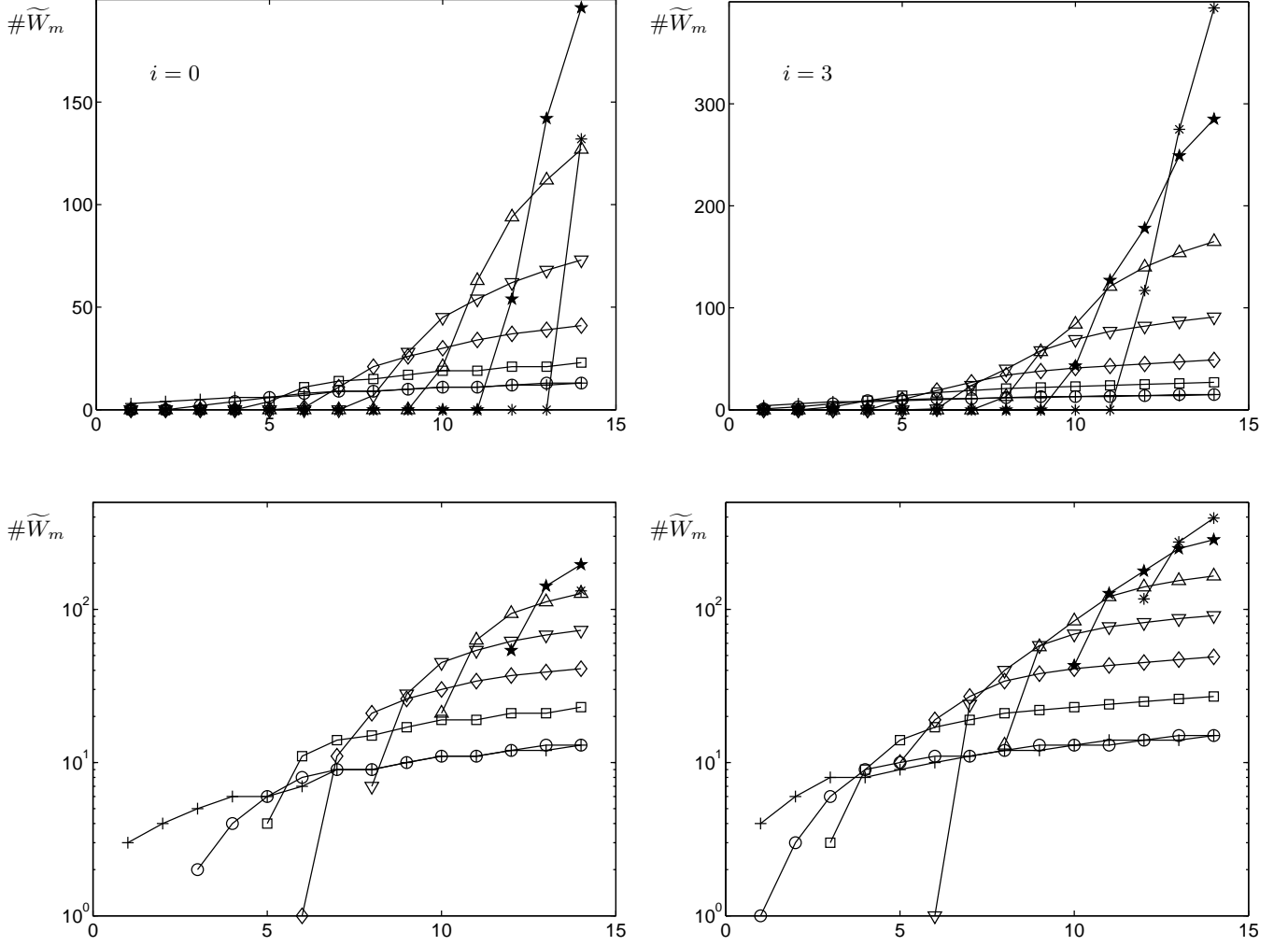


FIG. 2: The number of the significant basis functions in various subspaces required to reproduce the $\|P_0\Psi_i\|^2$ and $\|Q_m\Psi_i\|^2$ to a given precision. The horizontal axis shows the number of digit 9 in the threshold value η . The sign + stands for the restricted scaling function subspace \widetilde{V}_0 , whereas the signs \circ , \square , \diamond , ∇ , \triangle , \star and $*$ denote the detail spaces \widetilde{W}_m , with $m=0, 1, 2, 3, 4, 5, 6$, respectively. The results for the ground state ($i=0$) are plotted in the left column both in linear and log scale, while the right column corresponds to the third excited state.

task, and for exactly determining the integrals of products of scaling function derivatives [11]. Finally, the Hamiltonian matrix was diagonalized by standard subroutines.

At each refinement level (granularity) M the diagonalization of the Hamiltonian matrix $H|_{\mathcal{H}^{[M]}}$ restricted to the appropriate subspace $\mathcal{H}^{[M]}$ leads to the eigenvector components $c_{0\ell}^{[M]}$ and $d_{m\ell}^{[M]}$, which are the expansion coefficients of

$$\Psi^{[M]}(x) = \sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} s_{0\ell}(x) + \sum_{m=0}^{M-1} \sum_{\ell \in \mathbb{Z}} d_{m\ell}^{[M]} w_{m\ell}(x) \quad (12)$$

for the approximate eigenstates. As the basis set of $\mathcal{H}^{[M]} = \mathcal{H}^{[M-1]} \oplus W_{M-1}$ is an extension to that of $\mathcal{H}^{[M-1]}$, the expansion coefficients resulted from independent diagonalizations of $H|_{\mathcal{H}^{[M-1]}}$ and $H|_{\mathcal{H}^{[M]}}$ can change in the refinement step $M-1 \rightarrow M$. Describing the trajectory of $\Psi^{[M]}$ in \mathcal{H} in terms of the granularity, would need to trace all the coefficients $c_{0\ell}^{[M]}$ and $d_{m\ell}^{[M]}$, this is however, hard to demonstrate. Instead, we have collected the ground state projections to a given detail space, and presented them in Tab. I. The excellent convergence can be easily realized. After few refinement steps the coefficients stabilize.

For higher excitations the overall trend is similar to that illustrated in Tab. I for the ground state, with the remark, that the contributions of finer detail spaces are more and more emphasized for increasing excitation levels. As an illustration, we recall the projections of the $i = 3$ excited state to the wavelet subspaces at resolution level $M = 5$: $\|P_0\Psi_3^{[5]}\|^2 = 0.86367$, $\|Q_0\Psi_3^{[5]}\|^2 = 0.13284$, $\|Q_1\Psi_3^{[5]}\|^2 = 3.4188 \times 10^{-3}$, $\|Q_2\Psi_3^{[5]}\|^2 = 6.5664 \times 10^{-5}$, $\|Q_3\Psi_3^{[5]}\|^2 = 1.0810 \times 10^{-6}$ and $\|Q_4\Psi_3^{[5]}\|^2 = 1.7114 \times 10^{-8}$.

For completeness, we have also given the errors of the ground and excited state energy approximations in the Hilbert spaces $\mathcal{H}^{[M]}$ in Fig. 3. Exponential convergence in terms of the granularity level M can be clearly identified.

IV. AN ADAPTIVE METHOD FOR DETERMINING FINE STRUCTURE LOCALIZATION REGIONS

In realistic cases, of course, exact solutions of the eigenvalue problem are not known. We can suppose, however, that quantum mechanical systems behave similarly to the simple exact case studied above. We expect, that high resolution wavelets can completely be omitted, and even at lower resolutions only a fractional part of them contribute essentially to the expansion. In the following considerations we will apply a consistent notation for the two distinct truncation schemes. Upper index $[M]$ denotes the “vertical” cutoff of the Hilbert space above the granularity M , whereas tilde is applied to indicate the “horizontal” truncation in a given detail space W_m .

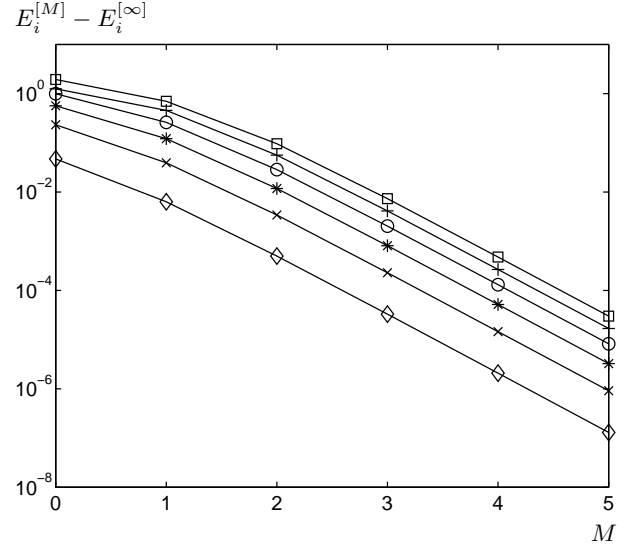


FIG. 3: The errors of the approximate energies $E_i^{[M]}$ determined in the Hilbert space $\mathcal{H}^{[M]}$. The sign \diamond stands for the ground state $i = 0$, whereas the signs \times , $*$, \circ , $+$ and \square denote the excitations $i = 1, 2, 3, 4, 5$, respectively. Atomic units are used.

Our goal is to develop a method for determining the significant coefficients in (1), without calculating all the negligible ones. This requires predicting the set of important fine level coefficients for $M + 1$, supposing that the approximate expansion

$$\tilde{\Psi}^{[M]}(x) = \sum_{\ell \in \tilde{V}_0} \tilde{c}_{\ell}^{[M]} s_{0\ell}(x) + \sum_{m=0}^{M-1} \sum_{\ell \in \tilde{W}_m} \tilde{d}_{m\ell}^{[M]} w_{m\ell}(x). \quad (13)$$

of the wave function is already known. Here, we have used the loose notation $\ell \in \tilde{W}_m$, indicating the fact, that the summation index ℓ is constrained to the wavelets $w_{m\ell}$ which belong to the restricted subspace \tilde{W}_m . In the first summation \tilde{V}_0 denotes the restricted subspace of those scaling functions which are localized in the finite domain of the space, which is occupied by the system.

The iterative extension $\tilde{\Psi}^{[M]} \rightarrow \tilde{\Psi}^{[M+1]}$ can be separated to two independent problems. The first step is determining the significant part \tilde{W}_M of the M th level detail space, knowing the approximation $\tilde{\Psi}^{[M]}$. In the other step, the numerical determination of the expansion coefficients $\tilde{d}_{M\ell}$ in \tilde{W}_M should be carried out. In this work, we will concentrate on the solution of the first problem. In order to distinguish the errors emerging from different sources, the second part of the calculation is carried out by an exact diagonalization of the Hamiltonian $\tilde{H}^{[M+1]}$ restricted to the subspace $\tilde{\mathcal{H}}^{[M+1]} = \tilde{V}_0 \oplus \tilde{W}_0 \oplus \dots \oplus \tilde{W}_M$. In optimized numerical works sophisticated methods for solving the eigenproblem of sparse matrices can be applied.

As $\tilde{\Psi}^{[M]}$ is the eigenfunction of the restricted Hamil-

TABLE I: The trajectory of the ground state wave function in the detail spaces V_0, W_0, \dots, W_4 : the contribution of the detail spaces to the M th coarse-grained approximations of the ground state eigenfunction. The last column shows the sum of the first five terms in Parseval's equation (4). In finite subspaces $\mathcal{H}^{[0]}, \dots, \mathcal{H}^{[5]}$ the relation fulfills exactly, whereas in the infinitely fine Hilbert space the error is of order 10^{-12} .

| M | $\ P_0\Psi_0^{[M]}\ ^2$ | $\ Q_0\Psi_0^{[M]}\ ^2$ | $\ Q_1\Psi_0^{[M]}\ ^2$ | $\ Q_2\Psi_0^{[M]}\ ^2$ | $\ Q_3\Psi_0^{[M]}\ ^2$ | $\ Q_4\Psi_0^{[M]}\ ^2$ | Sum |
|----------|-------------------------|----------------------------|---------------------------|----------------------------|---------------------------|--------------------------|--|
| 0 | 1 | | | | | | 1 |
| 1 | 0.997552283 | 2.4477165×10^{-3} | | | | | 1 |
| 2 | 0.997257786 | 2.6805076×10^{-3} | 6.170620×10^{-5} | | | | 1 |
| 3 | 0.997234805 | 2.7016396×10^{-3} | 6.247610×10^{-5} | 1.0791337×10^{-6} | | | 1 |
| 4 | 0.997233338 | 2.7030347×10^{-3} | 6.252997×10^{-5} | 1.0801295×10^{-6} | 1.731278×10^{-8} | | 1 |
| 5 | 0.997233246 | 2.7031230×10^{-3} | 6.253341×10^{-5} | 1.0801932×10^{-6} | 1.731382×10^{-8} | 2.7227×10^{-10} | 1 |
| ∞ | 0.997233239 | 2.7031289×10^{-3} | 6.253364×10^{-5} | 1.0801974×10^{-6} | 1.731389×10^{-8} | 2.7227×10^{-10} | $\dots \quad 1 - 4.34 \times 10^{-12}$ |

tonian $\tilde{H}^{[M]} = H|_{\tilde{\mathcal{H}}^{[M]}}$, it satisfies the equation

$$(\tilde{H}^{[M]} - \tilde{E}^{[M]})\tilde{\Psi}^{[M]} = 0. \quad (14)$$

This condition does not hold, if either $\tilde{H}^{[M]}$ or $\tilde{E}^{[M]}$ are replaced by their exact counterparts, and the quality of the M th resolution level approximate solution of the eigenvalue problem can be characterized by the error function

$$(H - \tilde{E}^{[M]})\tilde{\Psi}^{[M]} \neq 0. \quad (15)$$

Based on the methods developed in [9, 12], we suggest the following criterion for selecting the important basis functions of W_M . The error function (15) will be measured in the extended Hilbert space $\mathcal{H}^{[M+1]}$ (instead of the full Hilbert space \mathcal{H}). Considering, that according to (14) the expansion coefficients of the error function $\langle w_{m\ell} | (H - \tilde{E}^{[M]})\tilde{\Psi}^{[M]} \rangle = 0$ if $w_{m\ell} \in \tilde{\mathcal{H}}^{[M]}$, the magnitude of the deviation from the exact eigenvalue problem can be characterized by the magnitude of the expansion coefficients in the detail space W_M

$$r_{M\ell} = |\langle w_{M\ell} | H - \tilde{E}^{[M]} | \tilde{\Psi}^{[M]} \rangle|^2. \quad (16)$$

The wavelet $w_{M\ell}$ is considered to be “important” if $r_{M\ell}$ is larger than a given threshold. This test, however, can not be carried out in a reasonable time for all the basis functions in W_M , as this would require an exponential amount of work. Here, we apply an *adaptive* approach. We test the wavelets $w_{M\ell}$ only for those values of ℓ , where the support of $w_{M\ell}$ overlaps with the previously found “important region” of W_{M-1} .

To be more specific, we apply the following procedure.

1. We select a preliminary set \widehat{W}_M of wavelets $w_{M\ell}$ for which the condition

$$\text{support}(w_{M\ell}) \cap \text{support}(\widehat{W}_{M-1}) \neq \emptyset$$

holds.

2. For the selected wavelets the values of (16) are calculated and the wavelets are sorted according to descending order of $r_{M\ell}$.
3. The first most important wavelets constituting the restricted subspace \widetilde{W}_M are kept until the condition

$$\sum_{\ell \in \widetilde{W}_M} r_{M\ell} - \sum_{\ell \in \widehat{W}_M} r_{M\ell} \leq 1 - \eta, \quad (17)$$

similar to (8) is fulfilled. Depending on the required precision η the set \widetilde{W}_M is usually much smaller than the candidate set \widehat{W}_M .

The adaptive fine structure localization method reduces the size of the detail spaces considerably, for example, in the case of nine-9 precision ($\eta = 0.999999999$) and

the ground state wave function, $\dim W_6 = 646$, whereas $\dim \widetilde{W}_6 = 296$.

The results obtained for the wave function with various precision requirements η are summarized in Tables II and III. The wave function $\tilde{\Psi}^{[M]}$ calculated in the “horizontally” truncated Hilbert space is expected to significantly deviate from the eigenstate $\Psi^{[M]}$ received without truncation if the required precision is low. On the other hand, in the $\eta \rightarrow 1$ limit $\tilde{\Psi}^{[M]}$ approximates $\Psi^{[M]}$ very well.

Tab. II contains the deviations $\Delta \|P_0 \tilde{\Psi}_0^{[M]}\|^2 = \|P_0 \tilde{\Psi}_0^{[M]}\|^2 - \|P_0 \Psi_0^{[M]}\|^2$ and $\Delta \|Q_m \tilde{\Psi}_0^{[M]}\|^2 = \|Q_m \tilde{\Psi}_0^{[M]}\|^2 - \|Q_m \Psi_0^{[M]}\|^2$ for a rough precision $\eta = 0.99$. It can be seen, that the error of the wave function saturates with increasing resolution level M . The value of the error is significantly larger than the error caused by the “vertical” truncation of the Hilbert space.

Tab. III shows similar data for a moderate precision requirement $\eta = 0.9999999$. In this case the wave function $\tilde{\Psi}^{[M]}$, obtained using the adaptive fine structure localization method, gives an excellent approximation to $\Psi^{[M]}$. The error introduced by the “horizontal” truncation is less, than that of the “vertical” one, up to the resolution level $M = 5$.

In case of excited states, the eigenstates of the eigenvalue problem in granular Hilbert spaces with a given granularity M are less accurate than the ground state. The deviations due to “horizontal” truncation of the detail spaces, however, only slightly exceed the ground state values. Consequently, for a given M , the precision η which was appropriate for ground state calculations will certainly be applicable in excited state calculations, as well.

The errors of the approximate energies calculated for the ground and excited state $i = 3$ are plotted in Fig. 4 for various precision requirements η . For lower precision the magnitude of the error saturates at various resolution levels M , depending on the value of η . This fact, together with the observation concerning the error of the wave function, emphasizes the importance of choosing matching values for the precision requirement η and the granularity level M .

V. CONCLUSIONS

We have shown, that the fine structure of the Hilbert space vanishes exponentially in realistic wave functions. Realizing this fact, one can obtain excellent approximations of the eigenfunctions by omitting the fine resolution detail spaces and solving the eigenvalue problem in granular Hilbert spaces. We have traced the trajectories of the approximate wave functions of an exactly solvable model system, and concluded, that they approach the exact wave function exponentially fast. A similar statement is valid for the approximate energy values.

A further possibility for reducing the computational

TABLE II: The deviation of the trajectory of $\tilde{\Psi}_0^{[M]}$ from that of $\Psi_0^{[M]}$ due to fine structure localization with $\eta = 0.99$ in the detail spaces V_0, W_0, \dots, W_4 .

| M | $\Delta \ P_0 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_0 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_1 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_2 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_3 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_4 \tilde{\Psi}_0^{[M]}\ ^2$ |
|-----|---|---|---|---|---|---|
| 1 | 0.41770×10^{-5} | 0.41770×10^{-5} | | | | |
| 2 | 3.22557×10^{-5} | 3.22325×10^{-5} | -0.23237×10^{-7} | | | |
| 3 | 3.14686×10^{-5} | 3.17587×10^{-5} | 2.50837×10^{-7} | 3.92755×10^{-8} | | |
| 4 | 2.76469×10^{-5} | 2.82869×10^{-5} | 5.95967×10^{-7} | 4.31415×10^{-8} | 0.89745×10^{-9} | |
| 5 | 2.75634×10^{-5} | 2.81104×10^{-5} | 5.11324×10^{-7} | 3.44685×10^{-8} | 1.19115×10^{-9} | 2.901×10^{-11} |

TABLE III: The deviation of the trajectory of $\tilde{\Psi}_0^{[M]}$ from that of $\Psi_0^{[M]}$ due to fine structure localization with $\eta = 0.999999$ in the detail spaces V_0, W_0, \dots, W_4 .

| M | $\Delta \ P_0 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_0 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_1 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_2 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_3 \tilde{\Psi}_0^{[M]}\ ^2$ | $\Delta \ Q_4 \tilde{\Psi}_0^{[M]}\ ^2$ |
|-----|---|---|---|---|---|---|
| 1 | -0.00209×10^{-9} | 0.00209×10^{-9} | | | | |
| 2 | 0.21649×10^{-9} | -0.21870×10^{-9} | 0.0220×10^{-10} | | | |
| 3 | -1.02284×10^{-9} | 1.04319×10^{-9} | -0.1999×10^{-10} | -0.036×10^{-11} | | |
| 4 | 4.15413×10^{-9} | -4.42360×10^{-9} | 2.9803×10^{-10} | -2.845×10^{-11} | -1.0×10^{-13} | |
| 5 | 3.26705×10^{-9} | -3.50721×10^{-9} | 2.6070×10^{-10} | -2.072×10^{-11} | 1.8×10^{-13} | -10^{-14} |

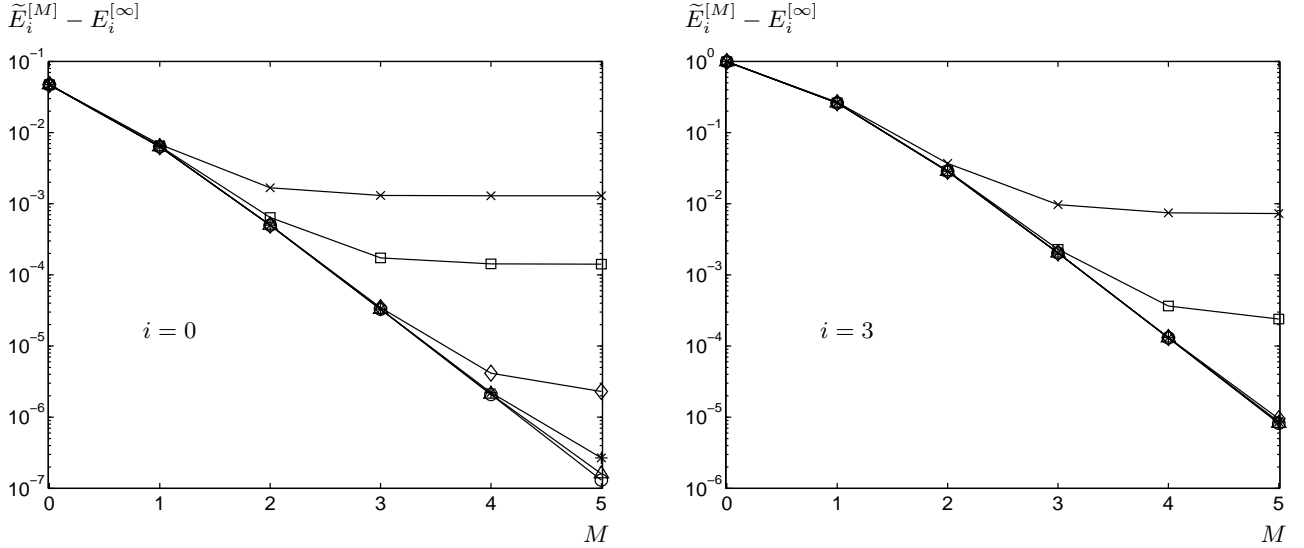


FIG. 4: The errors of the approximate energies $\tilde{E}_i^{[M]}$ determined in the Hilbert space $\tilde{\mathcal{H}}^{[M]}$ for the ground state $i = 0$ and for an excited state $i = 3$. The signs $\times, \square, \diamond, *, \triangle$ and \circ stand for the threshold values $\eta = 0.9, 0.99, 0.999, 0.9999, 0.99999$ and 0.999999 , respectively. Atomic units are used.

complexity of the calculations, that higher resolution wavelets are included in the basis set only in those spatial regions where the fine structure of the wave function requires it. For our model system we found, that the number of significant basis functions is considerably less than the dimension of the detail subspaces included in full calculations. The *a priori* selection of the significant basis functions needs a predictive algorithm.

Based on the above concept, we have developed an adaptive method for selecting the essential basis functions using the fine structure localization technique. Calculations in truncated Hilbert spaces, restricted in such manner lead to sufficiently precise wave functions and eigenenergies, even in the case of moderately strict basis function selection criterion.

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